Physical nature of all the electronic states in the Thue-Morse chain

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Abstract

We present an analytical method for finding all the electronic eigenfunctions and eigenvalues of the aperiodic Thue-Morse lattice. We prove that this system supports only extended electronic states which is a very unusual behavior for this class of systems, and so far as we know, this is the only example of a quasiperiodic or aperiodic system in which critical or localized states are totally absent in the spectrum. Interestingly we observe that the symmetry of the lattice leads to the existence of degenerate eigenstates and all the eigenvalues excepting the four global band edges are doubly degenerate. We show exactly that the Landauer resistivity is zero for all the degenerate eigenvalues and it scales as $\sim L^2$ (L = system size) at the global band edges. We also find that the localization length ξ is always greater than the system size.

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In recent years, intense theoretical activities have been observed in the literature towards the understanding of the electronic properties of quasiperiodic and aperiodic systems. It has been seen that apart from the usual generic features like the critical wave functions, singular continuous energy spectrum, scaling properties of the density of states, power-law behavior of electrical conductivity etc. [1–3], these systems can also sustain many features characteristic of periodic as well as disordered systems. As for example, in a very recent work Maciá and Domínguez-Adame [4] have reported a new class of energy eigenstates in the spectrum of 1D quasiperiodic Fibonacci lattice having properties characteristic of extended electronic states. But Fibonacci lattice is the simplest and the most well-studied quasiperiodic model system since the discovery of icosahedral symmetry in Al-Mn alloy by Shechtman et al. [5] and the general consensus about its electronic structure is that all the eigenstates are critical with Cantor-set energy spectrum. This kind of diversity of the electronic and other properties are the general characteristics of almost every quasiperiodic or aperiodic system. A few such instances are the period-doubling [6,7], copper-mean [8], Rudin-Shapiro [9] and Thue-Morse [10,11] etc. lattices and in these systems critical as well as extended wave functions can coexist. Moreover, in some of these cases there is evidence of localized [12] or chaotic wave functions [13]. There are also notions like the self-similar, lattice-like or Bloch-like wave functions regarding the nature of the eigenstates. The associated spectra can be absolutely continuous, singular continuous or point singularities, and in many cases the spectra seem to be a mixture of these possibilities. All these information lead to a somewhat confusing situation, and these controversies can be resolved only if one has clear knowledge of every eigenvalue and eigenfunction of the system. The analytical answer to this problem is not very straightforward and in general, every quasiperiodic or aperiodic system needs separate attention.

As a first step, in this paper we shall provide an instance of an aperiodic system where we have succeeded in overcoming all the ambiguities in its electronic properties. This is the case of the well-known Thue-Morse lattice (TM), a deterministic aperiodic system whose Schrödinger equation has been analytically solved to give a full account of all its eigenval-

ues and eigenfunctions. Recent investigations on this system show that it exhibits many contrasting physical behaviors. The electronic properties of this lattice is more like those of periodic lattices than the quasiperiodic systems, while with regard to Fourier spectrum it has a degree of order intermediate between disorder and quasiperiodic lattices. The Fourier spectrum is singular continuous [14], whereas the phonon spectrum is Cantor-set like [15]. Even if we focus our attention only on the electronic properties of the TM lattice, there are a number of papers in the literature showing many apparently contradicting features. Using the dynamical trace-map [16] approach Ryu et al. [13] have provided numerical evidence for the existence of critical and extended states in the TM lattice within the tight-binding model. From their results it also appears that lattice-like and chaotic wave functions are possible in the system. La Rocca [17] performed a multifractal analysis of the system and suggested that the spectrum contains absolutely continuous parts (extended states) as well as point singularities (localized states). Huang et al. [12] have calculated the mean resistance of the TM system and claimed that it is more localized than the Fibonacci chain. In an interesting analytical work, Chakrabrarti et al. [10] have provided the restrictive conditions on the energy eigenvalues for which the TM lattice can support extended electronic states. They have shown that a definite type of short range correlation among the atoms is responsible for the existence of extended states in the TM lattice, and it is quite different from the well-known dimer-type correlation [18]. But this work does not provide any insight about the entire spectrum giving full details of all the eigenstates of the system. Thus it seems that a clear understanding of the electronic properties of the TM lattice is still lacking and the present paper intends to resolve it on the basis of rigorous mathematical and physical considerations.

The formalism we introduce is based on the dynamical trace-map [16] of the TM lattice and the commutation properties of the transfer matrices, and it provides a very simple analytical method for finding all the eigenvalues and eigenfunctions of the system. This is essentially a renormalization group approach and it gives a transparent picture of the nature of the states. The key point of this work is the association of the eigenvalues obtained by

the trace-map technique with the commutation properties of the transfer matrices and the underlying physical mechanism is as follows. We can consider the infinite TM lattice, at any length scale, as built up of two basic clusters and the transfer matrices for these clusters become identical at certain eigenvalues of the system. So we can map the aperiodic TM lattice effectively into a periodic lattice, and it explains why this lattice can support extended electronic eigenstates. Most surprisingly we observe that the TM lattice sustains *only* extended wavefunctions, a feature quite uncharacteristic of any quasiperiodic or aperiodic system. Also, we have shown exactly that the localization length ξ is always greater than the system size, which again signifies the delocalized character of all the states. Quite interestingly we have noticed that the symmetry of the TM lattice manifests itself in a beautiful way giving rise to the appearance of degenerate states in one-dimension within the tight-binding formalism. This a very unusual behavior for any one-dimensional tight-binding system where degenerate eigenstates are almost forbidden, and the TM lattice can be considered as an exception. We have seen that apart from the four eigenvalues corresponding to the global band edges, all other eigenvalues are doubly degenerate, and thus our work invalidates the findings of Cheng et al. [14]. To gain further insight about the nature of the states, we have also studied the transport properties of the electrons. We have derived exact expression for the Landauer resistivity of the lattice and shown that all the degenerate states exhibit Bloch-like behavior in the sense that the Landauer resistivity are zero for these states, while for the remaining four states the Landauer resistivity scales as $\sim L^2$, L being the length of the chain.

The TM sequence $\sigma_n(\bar{\sigma}_n)$ of order n may be generated by starting with the symbol $A(B)$ and applying the inflation rule $A \rightarrow AB$ and $B \rightarrow BA$ n-times recursively. It is easy to see that $\bar{\sigma}_n$ is the complement of σ_n obtained by interchanging A and B in σ_n, and they satisfy the recursion relations $\sigma_{n+1} = \sigma_n\bar{\sigma}_n$ and $\bar{\sigma}_{n+1} = \bar{\sigma}_n\sigma_n$. Now one can construct a TM chain by considering the symbols A and B representing two atoms A and B. The electronic properties of such a lattice are generally modelled by the on-site version of the nearest neighbor tight-binding Hamiltonian and the corresponding Schrödinger equation in

Wannier basis is given by

$$(E - \epsilon_i)\psi_i = \psi_{i+1} + \psi_{i-1} \ , \tag{1}$$

where ψ_i is the amplitude of the wave function at the ith site, $\epsilon_i = \epsilon_A$ or ϵ_B, and t is the hopping integral being set to unity. Now first we solve the Eqs. (1) for the nth generation chain with the periodic boundary condition, and then consider the limit $n \to \infty$ for finding the electronic structure of the infinite lattice (see Ref. [19]). Using the transfer matrix method we now show that all the eigenvalues of the TM chain can be obtained from its trace-map [16], which satisfies the relation

$$\alpha_{n+1} = 4\alpha_{n-1}^2(\alpha_n - 1) + 1 \qquad \text{for} \ \ n \geq 2, \tag{2}$$

where $\alpha_n = (\mathrm{Tr}M_n)/2$, M_n being the transfer matrix of the nth generation TM lattice. If we choose the origin of energy in such a way that $\epsilon_A = -\epsilon_B = V$, then the initial conditions are $\alpha_1 = (E^2 - V^2 - 2)/2$ and $\alpha_2 = 2\alpha_1^2 - 2V^2 - 1$. We see that α_n is a polynomial in E of degree 2^n, and for periodic boundary condition the relation $\alpha_n = 1$ determines all the 2^n eigenvalues of the nth generation chain consisting of $N = 2^n$ atoms. Let us now recast the trace-map Eq. (2) into the following form

$$\alpha_n = 4^{n-2}\alpha_{n-2}^2\alpha_{n-3}^2 \cdots \alpha_2^2\alpha_1^2(\alpha_2 - 1) + 1. \tag{3}$$

This form of the trace-map is quite suggestive and gives a lot of information about the spectrum. The eigenvalues of the system are given by the roots of the equations

$$\alpha_1^2 = \alpha_2^2 = \quad \cdots \quad = \alpha_{n-2}^2 = 0 \quad \text{and} \quad \alpha_2 - 1 = 0. \tag{4}$$

The equation $\alpha_2 - 1 = 0$ actually determines the global band edges [20], because the energies for which $\alpha_2 > 1$ are disallowed as it implies that $\alpha_n > 1$. The global band edges are situated at $E = \pm(\sqrt{V^2 + 1} \pm 1)$, and Eqs. (4) show that these are the only four non-degenerate eigenvalues in the spectrum of the TM chain. It is clear from the rest of the equations in (4) that all the other eigenvalues are doubly degenerate. The form of Eq. (3) also suggests

that these degenerate eigenvalues are all distinct. This is due to the fact that α_n cannot have any of the earlier α_i's (with $i < n$) as its factor. From the structure of Eq. (3) it is obvious that the spectrum of the nth generation TM lattice contains all the eigenvalues of every preceding lower generation chains. In other words, the eigenvalues of any arbitrary generation TM lattice remain as eigenvalues in all the succeeding higher generation chains, and by the method of induction they also belong to the spectrum of the infinite TM lattice. In practice, the spectrum of the infinite lattice can be obtained by making the generation number n sufficiently large, and we get two global bands (symmetric around $E = 0$) where all the eigenvalues are doubly degenerate excepting those corresponding to the four global band edges.

Knowing all the eigenvalues of the TM lattice, let us now look into the nature of the eigenstates of the system. From the symmetry of the TM sequence, we observe that the infinite lattice can be built up from every pair of unit cells of the form $(\sigma_n, \bar{\sigma}_n)$, where $\sigma_n(\bar{\sigma}_n)$ is the nth generation TM sequence. If we define the corresponding pair of transfer matrices as $(T_n, \bar{T}_n)$, then in the basis of (2×2) identity matrix I and three Pauli matrices σ_x, σ_y and σ_z both T_n and $\bar{T}_n$ can be expressed into the following form:
For odd n $(n \geq 3)$, we have

$$\begin{aligned} T_n &= \alpha_n I + \beta_n \sigma_x + \gamma_n \sigma_y + \delta_n \sigma_z \ , \\ \bar{T}_n &= \alpha_n I - \beta_n \sigma_x + \gamma_n \sigma_y + \delta_n \sigma_z \ , \end{aligned} \tag{5}$$

where the coefficients satisfy the recursion relations

$$\begin{aligned} \alpha_n &= \alpha_{n-2}^4 + \beta_{n-2}^4 + \gamma_{n-2}^4 + \delta_{n-2}^4 + 2(\gamma_{n-2}^2 + \delta_{n-2}^2) \\ &\quad \times (3\alpha_{n-2}^2 + \beta_{n-2}^2) + 2(\gamma_{n-2}^2 \delta_{n-2}^2 - \alpha_{n-2}^2 \beta_{n-2}^2) \ , \\ \beta_n &= 8\alpha_{n-2}\beta_{n-2}(\gamma_{n-2}^2 + \delta_{n-2}^2) \ , \\ \gamma_n &= 4(\alpha_{n-2}^2 - \beta_{n-2}^2 + \gamma_{n-2}^2 + \delta_{n-2}^2)\alpha_{n-2}\gamma_{n-2} \ , \\ \delta_n &= 4(\alpha_{n-2}^2 - \beta_{n-2}^2 + \gamma_{n-2}^2 + \delta_{n-2}^2)\alpha_{n-2}\delta_{n-2} \ , \end{aligned} \tag{6}$$

and the iteration starts from the set $\alpha_1 = 2ab - 1$, $\beta_1 = b - a$, $\gamma_1 = -i(a + b)$ and $\delta_1 = 2ab$, where $a = (E - V)/2$ and $b = (E + V)/2$.

For even n ($n \geq 4$), we get

$$\begin{aligned} T_n &= \alpha_n I + \gamma_n \sigma_y + \delta_n \sigma_z \ , \\ \bar{T}_n &= \alpha_n I + \gamma'_n \sigma_y + \delta'_n \sigma_z \ , \end{aligned} \tag{7}$$

and the recursion relations of the coefficients are given by

$$\begin{aligned} \alpha_n &= 4\alpha_{n-2}^2(\gamma_{n-2}\gamma'_{n-2} + \delta_{n-2}\delta'_{n-2}) + \\ &\qquad (\alpha_{n-2}^2 + \gamma_{n-2}^2 + \delta_{n-2}^2)(\alpha_{n-2}^2 + \gamma_{n-2}^{'2} + \delta_{n-2}^{'2}) \ , \\ \gamma_n &= \alpha_{n-2}(\theta_{n-2}\mu_{n-2} + \phi_{n-2}\nu_{n-2}) \ , \\ \delta_n &= \alpha_{n-2}(\phi_{n-2}\mu_{n-2} - \theta_{n-2}\nu_{n-2}) \ , \\ \gamma'_n &= \alpha_{n-2}(\theta_{n-2}\mu_{n-2} - \phi_{n-2}\nu_{n-2}) \ , \\ \delta'_n &= \alpha_{n-2}(\phi_{n-2}\mu_{n-2} + \theta_{n-2}\nu_{n-2}) \ , \end{aligned} \tag{8}$$

where $\theta_{n-2} = 2(\gamma_{n-2} + \gamma'_{n-2})$, $\phi_{n-2} = 2(\delta_{n-2} + \delta'_{n-2})$, $\mu_{n-2} = \alpha_{n-2}^2 + \gamma_{n-2}\gamma'_{n-2} + \delta_{n-2}\delta'_{n-2}$ and $\nu_{n-2} = \gamma_{n-2}\delta'_{n-2} - \gamma'_{n-2}\delta_{n-2}$. Here the initial set for iteration is $\alpha_2 = \alpha_1^2 - \beta_1^2 + \gamma_1^2 + \delta_1^2$, $\gamma_2 = 2(\alpha_1\gamma_1 - i\beta_1\delta_1)$, $\delta_2 = 2(\alpha_1\delta_1 + i\beta_1\gamma_1)$, $\gamma'_2 = 2(\alpha_1\gamma_1 + i\beta_1\delta_1)$ and $\delta'_2 = 2(\alpha_1\delta_1 - i\beta_1\gamma_1)$.

First we consider the case of odd n. If we set $\beta_n = 0$ in Eqs. (5), then the matrices T_n and $\bar{T}_n$ become identical and this is exactly equivalent to the commutation relation $[T_{n-1}, \bar{T}_{n-1}] = 0$. The condition $\beta_n = 0$ implies that $\beta_{n-2} = \beta_{n-4} = \cdots = \beta_3 = 0$ (β_1 being non-zero) and thus it also guarantees the equality between T_m and $\bar{T}_m$ for every $m = 3,\ 5,\ 7,\ \cdots\ n$. It can be shown from Eqs. (5) and (6) that the condition $\beta_n = 0$ actually satisfies the eigenvalue equation $\alpha_n = 1$. In fact, we can reduce $\beta_n = 0$ as the set of equations $\alpha_1 = \alpha_3 = \alpha_5 = \ \cdots = \ \alpha_{n-2} = 0$ and $\gamma_1^2 + \delta_1^2 = 0$, and this is effectively a subset of the eigenvalue equation Eqs. (4) obtained by the trace-map technique. It may be noted that the equation $\gamma_1^2 + \delta_1^2 = 0$ is identical to the relation $\alpha_2 - 1 = 0$, which gives the global band edges. Now we show that the rest of the equations in (4) actually correspond to the equality of T_n and $\bar{T}_n$ for even values of n. From Eqs. (7) and (8) we see that T_n and $\bar{T}_n$ become identical when $\alpha_{n-2} = 0$, and this condition also satisfies the eigenvalue equation $\alpha_n = 1$. Finally, combining the results for odd and even n, we obtain the equations

$\alpha_1 = \alpha_2 = \cdots = \alpha_{n-2} = 0$ and $\gamma_1^2 + \delta_1^2 = 0$ as the conditions for the equality between T_m and $\bar{T}_m$, where $m = 3,\ 4,\ \cdots\ n$. It should be noticed that these equality conditions precisely give all the distinct eigenvalues of the system (see Eqs. (4)), though they cannot detect the degeneracy of the levels. Nevertheless, it actually proves that at every eigenvalue of the system, we can always find a pair of unit cells for the TM lattice which become identical so far as the electronic properties are concerned. Thus the aperiodic TM lattice effectively maps into various periodic lattices for energy eigenvalues of the system, and this is the physical reason why all electronic states of the TM lattice are extended in nature. The wave functions do not have any Bloch-like periodicity, but they are extended in the sense that the amplitudes do not decay at infinity.

For the sake of illustration, in Fig.1 we display $|\psi_n|^2$ as a function of the site index n for a few selected energies. Here we have used the initial conditions $\psi_1 = \psi_0 = 1$ which is consistent with the periodic boundary condition [19], and the figures clearly indicate the extended character of the wave functions. It is worth mentioning that we do not find any chaotic wave functions as reported in Ref. [13]. Normally the critical wave functions show power-law divergence [1], however, in the case of TM lattice all the states are well-behaved without any divergence at infinity. In Ref. [21] K. Iguchi has shown that the trace map Eq.(2) has no cycle, which implies that the TM lattice does not support power-law diverging states. It is also apparent from the above analysis that the transition from extended type states to critical or localized type states cannot be induced in the TM lattice by changing the Hamiltonian parameters, a behavior analogous to that of periodic systems.

Now we calculate the Landauer resistivity [3] ρ of the TM lattice. Since we can express the global transfer matrix M_n in the form M^m (where M = unit cell transfer matrix and m = total number of unit cells) corresponding to every eigenvalue of the system, it can be written in the close form

$$M_n = I \quad (\text{for } \alpha_n = 0,\, n = 1, 2, 3, \cdots) \,,$$
$$= \begin{pmatrix} 1 + m\delta_3 & -im\gamma_3 \\ im\gamma_3 & 1 - m\delta_3 \end{pmatrix} \quad (\text{for } \gamma_1^2 + \delta_1^2 = 0) \,,$$

By embedding a finite size TM chain in a periodic array of A type atoms connected by hopping integrals $t = 1$, we obtain the following expression for the Landauer resistivity [3],

$$\rho = 0 \quad (\text{when } \alpha_n = 0,\, n = 1, 2, 3, \cdots)$$
$$= m^2\delta_3^2 \tan^2(k/2) \quad (\text{when } \delta_1 = i\gamma_1)$$
$$= m^2\delta_3^2 \cot^2(k/2) \quad (\text{when } \delta_1 = -i\gamma_1) \,,$$

where the wave vector k is given by the relation $2t\cos k = E - \epsilon_A$. Thus we can further classify the states according to the transport properties of the electrons in the TM lattice. We see that all the degenerate states are Bloch-like in the sense that the Landauer resistivity is zero for these states, while the four states corresponding to the global band edges are not Bloch-like as in these cases $\rho \sim L^2$, L being the length of the chain ($L \equiv N = ma$, $a =$ unit cell length). The non-zero value of ρ at the band edges physically indicates a transition between exponentially localized (gap) and extended (band) regions [2].

Let us now calculate the localization length (ξ) of the TM lattice from the expression for the global transfer matrix M_n. The Lyapunov exponent [19] can be evaluated exactly from the formula $\gamma = \lim_{N\to\infty}[N^{-1} \ln ||M_n||]$, where $||\ ||$ is the modulus of the matrix. We observe that for all the states of system size N, the localization length always has the value $\xi \equiv 1/\gamma = N/\ln 2$, and it proves the absence of localization in the TM lattice [22]. So from the point of view of localization of the electrons all states behave identically, whereas in terms of their transport properties the band edge states behave quite differently from the other states.

To conclude, in this paper we have developed an analytical method which gives full information about the electronic structure of the TM lattice. We have shown that all the electronic states in the aperiodic TM chain are extended in nature, which is a very surprising and completely new result. Another interesting finding is that it is an instance of a tight-

binding one-dimensional system which supports degenerate eigenstates. In this formalism it is also possible to determine the Landauer resistivity and localization length of the system exactly. We hope that this method will provide a guideline for studying the electronic structure of systems of similar type.

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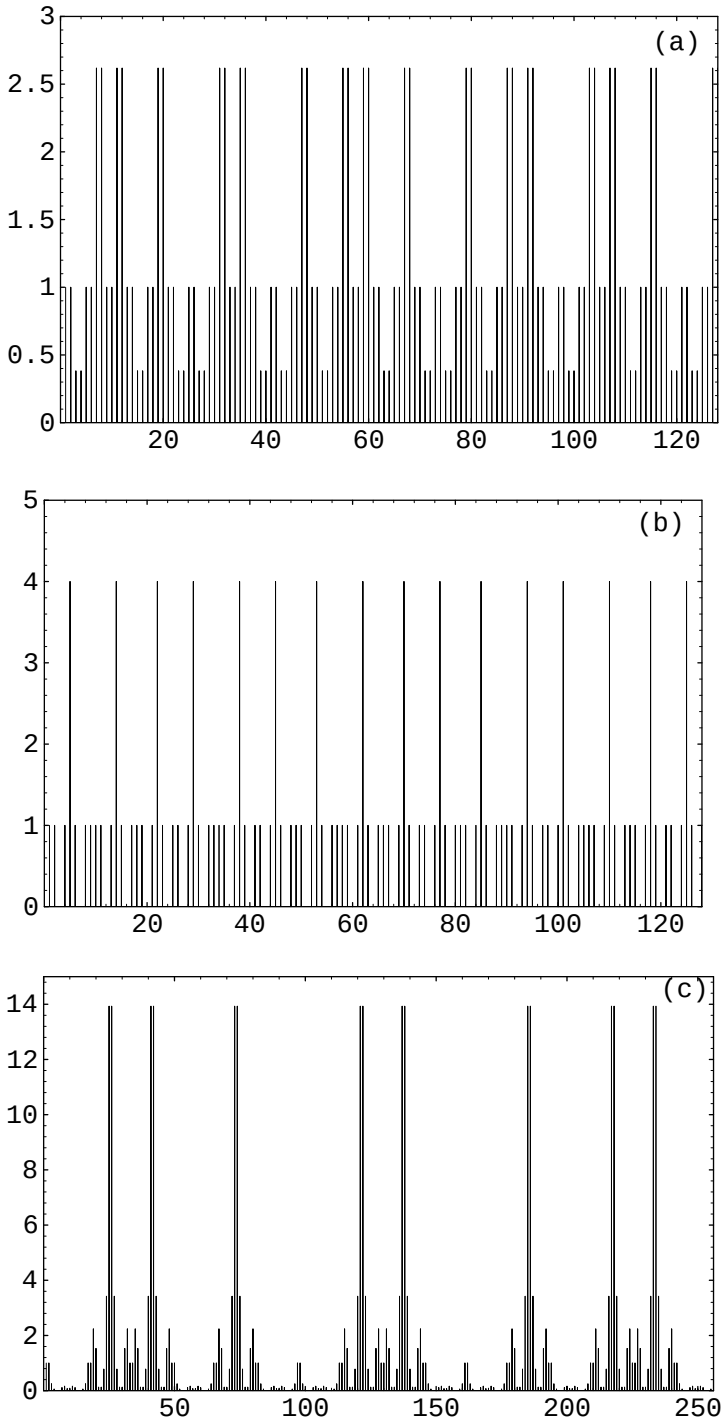
FIGURES

FIG. 1. Plot of $|\psi_n|^2$ versus site number n. Here $V = 0.5$ and (a), (b) and (c) correspond, respectively, to energies 2.1180339, 1.5 and 1.9955076. All energies are measured in units of hopping integral t.


(a)
3
2.5
2
1.5
1
0.5
0
20
40
60
80
100
120
(b)
5
4
3
2
1
0
20
40
60
80
100
120
(c)
14
12
10
8
6
4
2
0
50
100
150
200
250